

10/553451 CRYSTAL p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

=> d his

(FILE 'HOME' ENTERED AT 08:28:57 ON 15 JUN 2007)

FILE 'REGISTRY' ENTERED AT 08:29:10 ON 15 JUN 2007

L1 STRUCTURE UPLOADED
L2 0 S L1 SSS SAM
L3 3 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 08:31:07 ON 15 JUN 2007

L4 4 S L3

FILE 'REGISTRY' ENTERED AT 08:33:14 ON 15 JUN 2007

L5 1 S 61581-05-3/RN

FILE 'CAPLUS' ENTERED AT 08:33:56 ON 15 JUN 2007

L6 0 S L5 AND "TRANSITION TEMPERATURE"
L7 140091 S "TRANSITION TEMPERATURE"
L8 101545 S HYDRATE
L9 0 S L5 AND L8
L10 228517 S ANHYDRIDE
L11 2184 S L8 AND L10
L12 0 S L11 AND L5
L13 0 S L5 AND PRECIPITATION
L14 0 S L5 AND PRECIPITATING
L15 0 S L5/RGT
L16 0 S L5/PREP
L17 0 S L5/PROC
L18 0 S L5/PUR
L19 0 S L5 AND PARAHYDROXYBENZOIC

FILE 'CASREACT' ENTERED AT 08:47:29 ON 15 JUN 2007

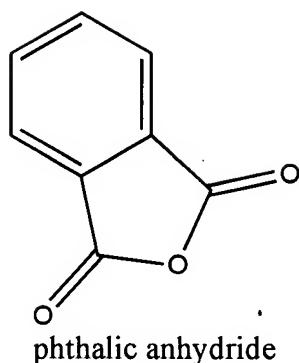
L20 0 S L5
 E L5
L21 193 S E3 OR E6

FILE 'CAPLUS' ENTERED AT 08:49:45 ON 15 JUN 2007

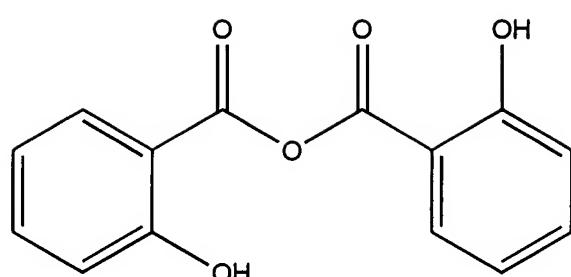
L22 193 S L21
L23 1 S L22 AND L7
L24 0 S L22 AND PRECIPITATING
L25 1 S L7 AND L22

FILE 'STNGUIDE' ENTERED AT 08:51:44 ON 15 JUN 2007

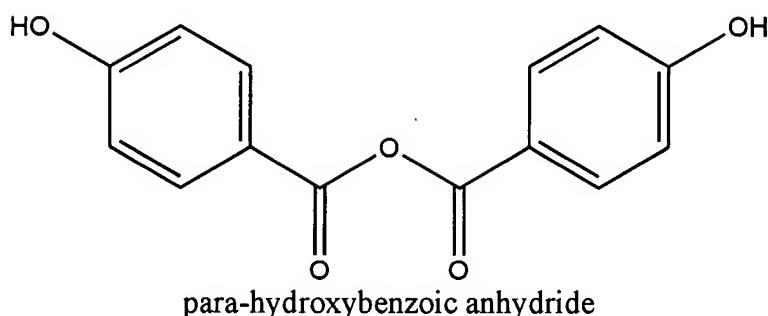
STN Search (add'l)
6/19/07
MM



phthalic anhydride

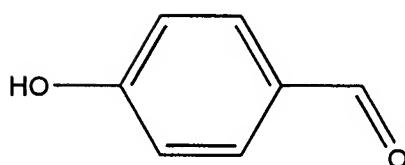


hydroxybenzoic anhydride



para-hydroxybenzoic anhydride

SN 10/553451



para-hydroxybenzoic acid monohydrate

=> e US20060264670/apps
E1 1 US2006-DS248308/PRN
E2 1 US2006-DS259834/PRN
E3 0 --> US20060264670/AP
E4 0 US20060264670/PRN
E5 1 US2007-528724/AP
E6 1 US2007-530406/AP
E7 1 US2007-530492/AP
E8 1 US2007-531465/AP
E9 1 US2007-532703/AP
E10 1 US2007-539995/AP
E11 1 US2007-541273/AP
E12 1 US2007-542249/AP

=> e US2006-264670/apps
E1 1 US2006-251648/AP
E2 1 US2006-256007/AP
E3 0 --> US2006-264670/AP
E4 0 US2006-264670/PRN
E5 1 US2006-264673/AP
E6 1 US2006-265883/AP
E7 1 US2006-271355/AP
E8 1 US2006-274942/AP
E9 1 US2006-275437/AP
E10 1 US2006-275438/AP
E11 1 US2006-275439/AP
E12 1 US2006-275453/AP

=> s US2006-264670/apps
0 US2006-264670/AP
0 US2006-264670/PRN
L26 0 US2006-264670/APPS
(US2006-264670/AP, PRN)

=> e US20060264670/apn,prn,pn
'APN' IS NOT A VALID EXPAND FIELD CODE FOR FILE 'CAPLUS'
E1 1 US2006026035/PN
E2 1 US2006026040/PN
E3 0 --> US20060264670/PRN
E4 0 US20060264670/PN
E5 1 US2006026610/PN
E6 1 US2006026622/PN
E7 1 US2006026694/PN
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E12 1 US2006026700/PN

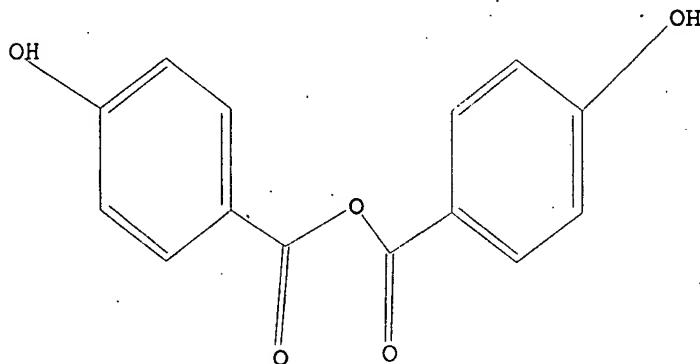
The indicated field code is not available for EXPAND in this file. To see a list of valid EXPAND field codes, enter HELP SFIELDS at an arrow prompt (>).

10/553451 CRYSTAL p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

=>
Uploading C:\Program Files\Stnexp\Queries\2007 cases\10553451\parahydroxybenzoic
anhydride.str

L1 STRUCTURE UPLOADED

=> d 11
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11 sss sam
SAMPLE SEARCH INITIATED 08:29:33 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 849 TO ITERATE

100.0% PROCESSED 849 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
PROJECTED ITERATIONS: 15232 TO 18728
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s 11 sss full
FULL SEARCH INITIATED 08:29:42 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 17618 TO ITERATE

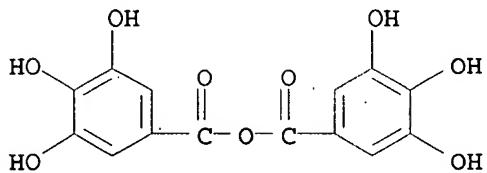
100.0% PROCESSED 17618 ITERATIONS 3 ANSWERS
SEARCH TIME: 00.00.01

L3 3 SEA SSS FUL L1

=> d scan

L3 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Benzoic acid, 3,4,5-trihydroxy-, anhydride (9CI)
MF C14 H10 O9

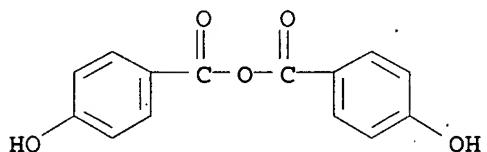
10/553451 CRYSTAL p-HYDROXYBENZOIC ACID ANHYDRIDE - structure



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

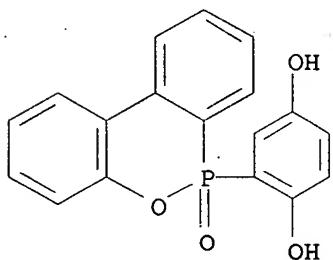
L3 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Benzoic acid, 4-hydroxy-, anhydride (9CI)
MF C14 H10 O5
CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

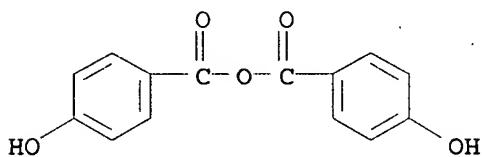
L3 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 1,4-Benzenedicarboxylic acid, polymer with 4-hydroxybenzoic acid anhydride
and 2-(6-oxido-6H-dibenz[c,e][1,2]oxaphosphorin-6-yl)-1,4-benzenediol
(9CI)
MF (C18 H13 O4 P . C14 H10 O5 . C8 H6 O4)x
CI PMS

CM 1

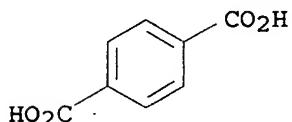


CM 2

10/553451 CRYSTAL p-HYDROXYBENZOIC ACID ANHYDRIDE - structure



CM 3



ALL ANSWERS HAVE BEEN SCANNED

=> fil caplus
COST IN U.S. DOLLARS
FULL ESTIMATED COST

| SINCE FILE ENTRY | TOTAL SESSION |
|------------------|---------------|
| 173.00 | 173.21 |

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FILE COVERS 1907 - 15 Jun 2007 VOL 146 ISS 25
FILE LAST UPDATED: 13 Jun 2007 (20070613/ED)

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=> d his

(FILE 'HOME' ENTERED AT 08:28:57 ON 15 JUN 2007)

FILE 'REGISTRY' ENTERED AT 08:29:10 ON 15 JUN 2007
L1 STRUCTURE uploaded
L2 0 S L1 SSS SAM
L3 3 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 08:31:07 ON 15 JUN 2007

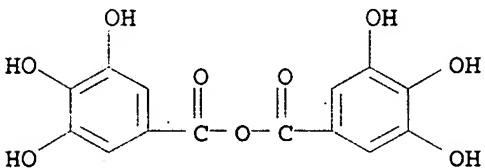
=> s 13
 L4 4 L3

=> d ibib abs 14 1-4 hitstr

L4 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2004:328553 CAPLUS
 DOCUMENT NUMBER: 141:64396
 TITLE: A comparative study of quantitative structure-activity
 relationship methods based on gallic acid derivs.
 Huang, H.; Ou, W.; Zhao, J.; Chen, D.; Wang, L.
 CORPORATE SOURCE: State Key Lab. Pollution Control and Resources Reuse,
 Sch. Environ., Nanjing Univ., Nanjing, Peop. Rep.
 China
 SOURCE: SAR and QSAR in Environmental Research (2004), 15(2),
 83-99
 CODEN: SQERED; ISSN: 1062-936X
 PUBLISHER: Taylor & Francis Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

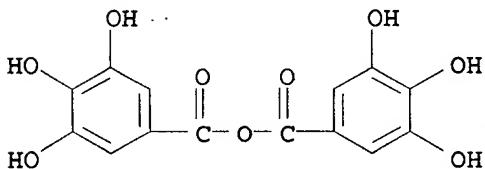
AB By using hologram quant. structure-activity relationship (HQSAR) and
 comparative mol. field anal. (CoMFA) methods, the relationships between
 the structures of 49 gallic acid derivs. and their analgesic activity have
 been investigated to yield statistically reliable models with considerable
 predictive power. The best HQSAR model was generated using atoms, bond
 and connectivity as fragment distinction parameters and fragment size 5-7
 from a hologram length of 307 with 3 components. High conventional r^2
 $(r^2=0.825)$ and cross-validation r^2 ($rcv^2=0.726$) values were obtained.
 CoMFA analyses varying lattice size and location, grid spacing, probe
 charges and using, Tripos standard and Indicator force field were performed.
 The best model was developed with 4 components using sp³-hybridized carbon
 atom with +1.0 charge as probe, grid spacing (2 Å), lattice offset
 $(1.0, 3.0, -2.5)$. The CoMFA model showed a conventional correlation
 coefficient r^2 of 0.889 and a cross-validation rcv^2 equals to 0.633. The
 robustness and predictive ability of the HQSAR and CoMFA models have been
 validated by means of an external test set. The results indicate that
 both models possess high statistical quality in the prediction of
 analgesic potency of novel gallic acid analogs.

IT 330664-37-4
 RL: PAC (Pharmacological activity); BIOL (Biological study)
 (comparative study of quant. structure-activity relationship methods
 based on gallic acid derivs.)
 RN 330664-37-4 CAPLUS
 CN Benzoic acid, 3,4,5-trihydroxy-, anhydride (9CI) (CA INDEX NAME)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2001:26712 CAPLUS
 DOCUMENT NUMBER: 134:231506
 TITLE: Structure-activity relationships for the analgesic activity of gallic acid derivatives
 AUTHOR(S): Krogh, R.; Yunes, R. A.; Andricopulo, A. D.
 CORPORATE SOURCE: College of Pharmacy, University of Michigan, Ann Arbor, MI, 48109, USA
 SOURCE: Farmaco (2000), 55(11-12), 730-735
 CODEN: FRMCE8; ISSN: 0014-827X
 PUBLISHER: Elsevier Science S.A.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Values of ID50 for a collection of structurally-related gallic acid derivs. have been employed to create a predictive quant. structure-activity relation (QSAR) which links structure to values of analgesic activity. The QSAR model developed has substantial predictive power for the design of novel gallic acid derivs. having improved analgesic potency.
 IT 330664-37-4
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (structure-activity relationships for analgesic activity of gallic acid derivs.)
 RN 330664-37-4 CAPLUS
 CN Benzoic acid, 3,4,5-trihydroxy-, anhydride (9CI) (CA INDEX NAME)



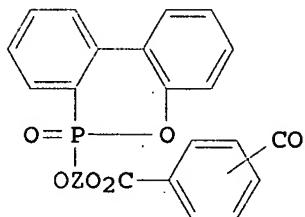
REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1987:619080 CAPLUS
 DOCUMENT NUMBER: 107:219080
 TITLE: Manufacture of aromatic polyester fibers
 INVENTOR(S): Matsumoto, Tetsuo; Makita, Hirotoshi; Kagawa, Yoshifumi
 PATENT ASSIGNEE(S): Japan Ester Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-------------|------|----------|-----------------|----------|
| ----- | ---- | ----- | ----- | ----- |
| JP 62177211 | A | 19870804 | JP 1986-17501 | 19860129 |

PRIORITY APPLN. INFO.: JP 1986-17501 19860129

GI



AB High-tenacity aromatic polyester fibers are prepared by melt spinning thermotropic liquid-crystal-formable aromatic polyesters containing 5-95 mol% I units (Z = trivalent aromatic group) at draft ratio ≥ 5 , passing the fibers through gas heated above the softening temperature (T_s) of the polyester, and finally passing them through gas heated above the glass transition temperature (T_g) of the polyester. Thus, a 2.5:7.5:2 (mole ratio) mixture of 9,10-dihydro-9-oxa-10-(2',5'-dihydroxyphenyl)phosphaphenanthrene 10-oxide (II), 4-hydroxybenzoic anhydride, and acetic anhydride and 1 mol/mol II terephthalic acid were copolymerd. to give an aromatic polyester (III). III (T_s 265°; T_g 186°) was spun at 330° and draft ratio 25, passed through gas at 275°, and subsequently passed through gas at 200° to give fibers with tenacity 14.7 g/denier and modulus 268 g/denier, vs. 2.8 g/denier and 205 g/denier, resp., for fibers spun at draft ratio 3.

IT 111523-01-4

RL: USES (Uses)

(fiber, melt spinning of, with high tenacity and modulus, draw ratio and heat-treatment temps. in relation to)

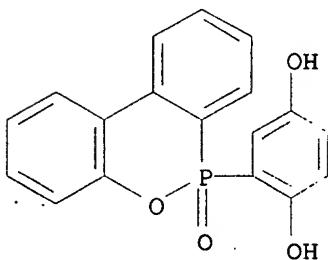
RN 111523-01-4 CAPLUS

CN 1,4-Benzenedicarboxylic acid, polymer with 4-hydroxybenzoic acid anhydride and 2-(6-oxido-6H-dibenz[c,e][1,2]oxaphosphorin-6-yl)-1,4-benzenediol (9CI) (CA INDEX NAME)

CM 1

CRN 99208-50-1

CMF C18 H13 O4 P

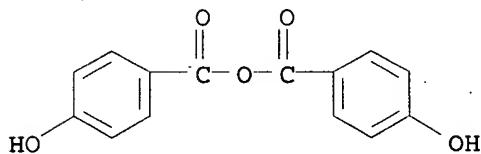


CM 2

CRN 61581-05-3

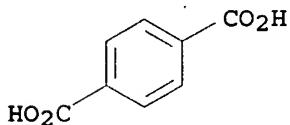
10/553451 CRYSTAL p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

CMF C14 H10 O5

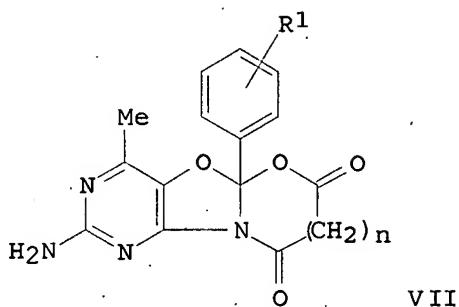
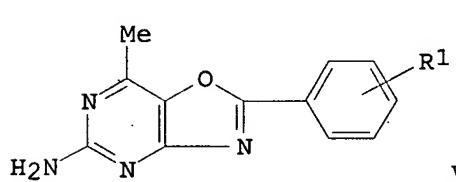
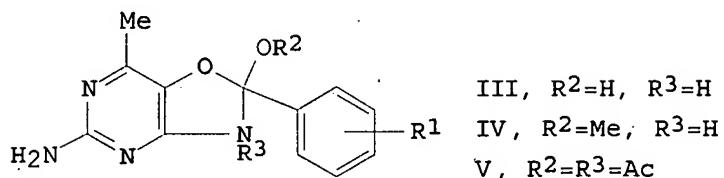
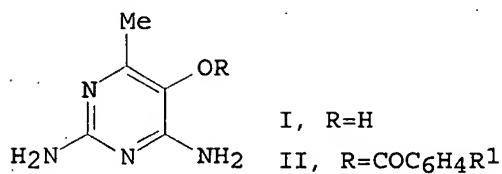


CM 3

CRN 100-21-0
CMF C8 H6 O4



L4 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1977:55385 CAPLUS
DOCUMENT NUMBER: 86:55385
TITLE: Synthesis of compounds related to antitumor agents.
IV. On the reaction of aromatic carboxylates with
2,4-diamino-5-hydroxy-6-methylpyrimidine
AUTHOR(S): Kato, Tetsuo; Oda, Noriichi; Ito, Issoo
CORPORATE SOURCE: Fac. Pharm. Sci., Nagoya City Univ., Nagoya, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1976), 24(10),
2461-9
DOCUMENT TYPE: CODEN: CPBTAL; ISSN: 0009-2363
LANGUAGE: Journal
GI English



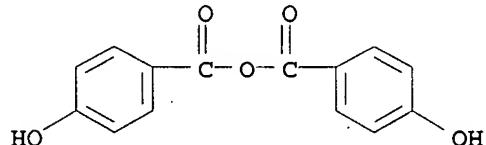
AB Reaction of the pyrimidine I with (R₁C₆H₄CO)₂O (R₁ = H, OH-o, -p, Me-o, -m, -p, NO₂-o, Cl-o) gave the corresponding II and the oxazolopyrimidines III. III were methylated (MeI), acetylated, dehydrated, or cyclized with ClCO(CH₂)_nCOCl (n = 1,2) to give IV-VII, resp.

IT 61581-05-3

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with diaminopyrimidinol)

RN 61581-05-3 CAPLUS

CN Benzoic acid, 4-hydroxy-, anhydride (9CI) (CA INDEX NAME)



=> fil reg
COST IN U.S. DOLLARS

| | |
|------------|---------|
| SINCE FILE | TOTAL |
| ENTRY | SESSION |

FULL ESTIMATED COST

22.96 196.17

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

| | |
|------------|---------|
| SINCE FILE | TOTAL |
| ENTRY | SESSION |

CA SUBSCRIBER PRICE

-3.12 -3.12

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10/553451 CRYSTAL p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

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STRUCTURE FILE UPDATES: 14 JUN 2007 HIGHEST RN 937362-79-3

DICTIONARY FILE UPDATES: 14 JUN 2007 HIGHEST RN 937362-79-3

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TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

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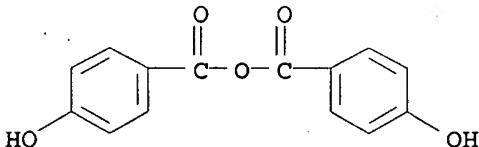
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> s 61581-05-3/rn
L5 1 61581-05-3/RN

=> d 15

L5 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN
RN 61581-05-3 REGISTRY
ED Entered STN: 16 Nov 1984
CN Benzoic acid, 4-hydroxy-, anhydride (9CI) (CA INDEX NAME)
OTHER NAMES:
CN p-Hydroxybenzoic acid anhydride
MF C14 H10 O5
CI COM
LC STN Files: CA, CAPLUS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

| => file caplu | SINCE FILE | TOTAL |
|--|------------|---------|
| COST IN U.S. DOLLARS | ENTRY | SESSION |
| FULL ESTIMATED COST | 2.40 | 198.57 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL |

10/553451 CRYSTALLOGRAPHY p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

CA SUBSCRIBER PRICE ENTRY 0.00 SESSION -3.12

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FILE COVERS 1907 - 15 Jun 2007 VOL 146 ISS 25
FILE LAST UPDATED: 13 Jun 2007 (20070613/ED)

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=> d his

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L1 STRUCTURE uploaded
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L3 3 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 08:31:07 ON 15 JUN 2007
L4 4 S L3

FILE 'REGISTRY' ENTERED AT 08:33:14 ON 15 JUN 2007
L5 1 S 61581-05-3/RN

FILE 'CAPLUS' ENTERED AT 08:33:56 ON 15 JUN 2007

=> s 15 and "transition temperature"

1 L5
988581 "TRANSITION"
264538 "TRANSITIONS"
1102834 "TRANSITION"
 ("TRANSITION" OR "TRANSITIONS")
628632 "TEMPERATURE"
81658 "TEMPERATURES"
697936 "TEMPERATURE"
 ("TEMPERATURE" OR "TEMPERATURES")
3068948 "TEMP"
779803 "TEMPS"
3408904 "TEMP"
 ("TEMP" OR "TEMPS")
3568308 "TEMPERATURE"

10/553451 CRYSTAL p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

("TEMPERATURE" OR "TEMP")
140091 "TRANSITION TEMPERATURE"
("TRANSITION" (W) "TEMPERATURE")
L6 0 L5 AND "TRANSITION TEMPERATURE"

=> s "transition temperature"
988581 "TRANSITION"
264538 "TRANSITIONS"
1102834 "TRANSITION"
("TRANSITION" OR "TRANSITIONS")
628632 "TEMPERATURE"
81658 "TEMPERATURES"
697936 "TEMPERATURE"
("TEMPERATURE" OR "TEMPERATURES")
3068948 "TEMP"
779803 "TEMPS"
3408904 "TEMP"
("TEMP" OR "TEMPS")
3568308 "TEMPERATURE"
("TEMPERATURE" OR "TEMP")
L7 140091 "TRANSITION TEMPERATURE"
("TRANSITION" (W) "TEMPERATURE")

=> s hydrate
86394 HYDRATE
28916 HYDRATES
L8 101545 HYDRATE
(HYDRATE OR HYDRATES)

=> s 15 and 18
1 L5
L9 0 L5 AND L8

=> s anhydride
217738 ANHYDRIDE
33390 ANHYDRIDES
L10 228517 ANHYDRIDE
(ANHYDRIDE OR ANHYDRIDES)

=> d his

(FILE 'HOME' ENTERED AT 08:28:57 ON 15 JUN 2007)

FILE 'REGISTRY' ENTERED AT 08:29:10 ON 15 JUN 2007
L1 STRUCTURE uploaded
L2 0 S L1 SSS SAM
L3 3 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 08:31:07 ON 15 JUN 2007
L4 4 S L3

FILE 'REGISTRY' ENTERED AT 08:33:14 ON 15 JUN 2007
L5 1 S 61581-05-3/RN

FILE 'CAPLUS' ENTERED AT 08:33:56 ON 15 JUN 2007
L6 0 S L5 AND "TRANSITION TEMPERATURE"
L7 140091 S "TRANSITION TEMPERATURE"
L8 101545 S HYDRATE
L9 0 S L5 AND L8

10/553451 CRYSTAL p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

L10 228517 S ANHYDRIDE

=> s l8 and l10

L11 2184 L8 AND L10

=> s l11 and l5

1 L5

L12 0 L11 AND L5

=> help operators

The following operators are available for use in searching: 'AND', 'OR', 'NOT', '(W)', '(NOTW)', '(A)', '(NOTA)', '(P)', '(NOTP)', '(S)', '(NOTS)', '(L)', '(NOTL)' and numeric operators. The order of precedence for the execution of operators is (highest first): numeric operators; '(W)', '(NOTW)', '(A)', and '(NOTA)'; '(S)' and '(NOTS)'; '(P)' and '(NOTP)'; '(L)' and '(NOTL)'; 'AND' and 'NOT'; then 'OR'. Parentheses (nesting) can be used to alter the order of execution. For example, the expression

=> SEARCH A AND B OR C NOT D

is equivalent to

=> SEARCH (A AND B) OR (C NOT D).

If the search logic required the set 'B OR C' to be combined with set A by 'AND' logic and set D by 'NOT' logic, parentheses would be required as shown below to produce the desired results.

=> SEARCH A AND (B OR C) NOT D

For more information on the individual operators, enter "HELP" and one of the following at an arrow prompt (=>): 'NUMERIC', '(NOTPROXIMITY)', 'AND', 'OR', 'NOT', '(W)', '(A)', '(S)', '(P)', or '(L)'. Information on specific negative proximity operators is found with the corresponding positive proximity operator; e.g., for information on '(NOTW)', enter "HELP (W)". The numeric, Boolean, and '(A)', '(NOTA)', '(W)', and '(NOTW)' word proximity operators work the same in all files. However, the function of the '(S)', '(NOTS)', '(P)', '(NOTP)', '(L)', and '(NOTL)' operators depends on the data structure of the file you are in. Entering "HELP (S)", "HELP (P)", or "HELP (L)" will give information about how these operators work in the current file.

=> d his

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L7 140091 S "TRANSITION TEMPERATURE"
L8 101545 S HYDRATE
L9 0 S L5 AND L8
L10 228517 S ANHYDRIDE
L11 2184 S L8 AND L10
L12 0 S L11 AND L5

=> s 15 and precipitation
1 L5
68195 PRECIPITATION
664 PRECIPITATIONS
68699 PRECIPITATION
(PRECIPITATION OR PRECIPITATIONS)
267038 PPTN
4375 PPTNS
269755 PPTN
(PPTN OR PPTNS)
291316 PRECIPITATION
(PRECIPITATION OR PPTN)
L13 0 L5 AND PRECIPITATION

=> s 15 and precipitating
1 L5
4403 PRECIPITATING
38040 PPTG
41350 PRECIPITATING
(PRECIPITATING OR PPTG)
L14 0 L5 AND PRECIPITATING

=> s 15/rgt
1 L5
46138 RGT/RL
L15 0 L5/RGT
(L5 (L) RGT/RL)

=> s 15/prep
1 L5
4417183 PREP/RL
L16 0 L5/PREP
(L5 (L) PREP/RL)

=> s 15/proc
1 L5
4118363 PROC/RL
L17 0 L5/PROC
(L5 (L) PROC/RL)

=> s 15/pur
1 L5
.257574 PUR/RL
L18 0 L5/PUR
(L5 (L) PUR/RL)

=> s 15 and parahydroxybenzoic
1 L5
61 PARAHYDROXYBENZOIC
L19 0 L5 AND PARAHYDROXYBENZOIC

=> fil casreact

10/553451 CRYs p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|--|------------------|---------------|
| FULL ESTIMATED COST | 36.94 | 235.51 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | 0.00 | -3.12 |

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FILE CONTENT: 1840 - 9 Jun 2007 VOL 146 ISS 25

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*
* CASREACT now has more than 12 million reactions *
*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 08:28:57 ON 15 JUN 2007)

FILE 'REGISTRY' ENTERED AT 08:29:10 ON 15 JUN 2007
L1 STRUCTURE UPLOADED
L2 0 S L1 SSS SAM
L3 3 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 08:31:07 ON 15 JUN 2007
L4 4 S L3

FILE 'REGISTRY' ENTERED AT 08:33:14 ON 15 JUN 2007
L5 1 S 61581-05-3/RN

FILE 'CAPLUS' ENTERED AT 08:33:56 ON 15 JUN 2007
L6 0 S L5 AND "TRANSITION TEMPERATURE"
L7 140091 S "TRANSITION TEMPERATURE"
L8 101545 S HYDRATE
L9 0 S L5 AND L8
L10 228517 S ANHYDRIDE
L11 2184 S L8 AND L10
L12 0 S L11 AND L5
L13 0 S L5 AND PRECIPITATION
L14 0 S L5 AND PRECIPITATING

10/553451 CRYSTALLOGRAPHY p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

L15 O S L5/RGT
L16 O S L5/PREP
L17 O S L5/PROC
L18 O S L5/PUR
L19 O S L5 AND PARAHYDROXYBENZOIC

FILE 'CASREACT' ENTERED AT 08:47:29 ON 15 JUN 2007

=> s 15
L20 O L5

=> e 15
E1 1 L4ZN8/BI
E2 1 L4ZNX2/BI
E3 166 --> L5/BI
E4 1 L50/BI
E5 1 L51784/BI
E6 27 L5178Y/BI
E7 1 L52/BI
E8 1 L5222/BI
E9 1 L52CU/BI
E10 1 L54MN4/BI
E11 1 L55/BI
E12 1 L56/BI

=> s e3 or e6
166 "L5"/BI
27 L5178Y/BI
L21 193 "L5"/BI OR L5178Y/BI

=> d scan

L21 193 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Extraction and coordination studies of the unexplored bifunctional ligand carbamoyl methyl sulfoxide (CMSO) with uranium(VI) and cerium(III) nitrates. Synthesis and structures of $[UO_2(NO_3)_2(\text{PhSOCH}_2\text{CONiBu}_2)]$ and $[\text{Ce}(\text{NO}_3)_3(\text{PhSOCH}_2\text{CONiBu}_2)_2]$
NO HIGHLIGHTING INFORMATION PRESENT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

L21 193 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Synthesis, coordination to Rh(I), and hydroformylation catalysis of new β -aminophosphines bearing a dangling nitrogen group: an unusual inversion of a Rh-coordinated P center
NO HIGHLIGHTING INFORMATION PRESENT

L21 193 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Sparsomycin analogs. V. Synthesis and antitumor activity of (E)- β -(pyrimidin-5-yl)acrylamides
NO HIGHLIGHTING INFORMATION PRESENT

L21 193 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Betaine-induced assembly of neutral infinite columns and chains of linked silver(I) polyhedra with embedded acetylenediide

10/553451 CRYSTAL p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

NO HIGHLIGHTING INFORMATION PRESENT

L21 193 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Cobalt(II) and manganese(II) complexes of unsymmetric compartmental ligands bearing adjacent {N,O} and {N,S,O} donor sets
NO HIGHLIGHTING INFORMATION PRESENT

L21 193 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Macrocyclic thioether-esters and thioether-thioesters and their palladium, platinum and silver complexes
NO HIGHLIGHTING INFORMATION PRESENT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> d 121 it

L21 ANSWER 1 OF 193 CASREACT COPYRIGHT 2007 ACS on STN

IT Michaelis constant
(kinetic parameters of protein kinases; preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen synthase kinase 3 inhibitors)

IT Crystal structure
Molecular structure
(of pyridocarbazole cyclopentadienylruthenium complex)

IT Human
(preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen synthase kinase 3 inhibitors)

IT 936112-70-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure; preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen synthase kinase 3 inhibitors)

IT 936112-68-4P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(mol. structure, HPLC chromatog. separation of isomers; preparation of

nitrogen
heterocyclic ruthenium metal complexes as glycogen synthase kinase 3 inhibitors)

IT 90698-26-3 114051-78-4, Lck kinase 137632-07-6, Erk1 kinase
141436-78-4, Protein kinase C α 144697-17-6, c-Src kinase
148047-34-1, ZAP-70 kinase 154907-65-0 391208-93-8, Glycogen synthase kinase 3 443900-95-6, Glycogen synthase kinase 3 β 553648-93-4,
Glycogen synthase kinase 3 α
RL: BCP (Biochemical process); BIOL (Biological study); PROC (Process)
(preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen synthase kinase 3 inhibitors)

IT 936232-98-3P 936233-00-0P
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);
PUR (Purification or recovery); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
(preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen synthase kinase 3 inhibitors)

IT 852658-41-4P 936112-65-1P 936112-66-2P 936112-69-5P
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);
SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

10/553451 CRYSTAL p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

(preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen synthase kinase 3 inhibitors)

IT 3724-16-1, 3-Pyridineacetamide 80049-63-4 259752-98-2 936112-71-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen synthase kinase 3 inhibitors)

IT 799822-53-0P 799822-54-1P 799822-55-2P 799822-56-3P 799822-57-4P

799822-58-5P 936112-67-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen synthase kinase 3 inhibitors)

=> d his

(FILE 'HOME' ENTERED AT 08:28:57 ON 15 JUN 2007)

FILE 'REGISTRY' ENTERED AT 08:29:10 ON 15 JUN 2007

L1 STRUCTURE uploaded

L2 0 S L1 SSS SAM

L3 3 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 08:31:07 ON 15 JUN 2007

L4 4 S L3

FILE 'REGISTRY' ENTERED AT 08:33:14 ON 15 JUN 2007

L5 1 S 61581-05-3/RN

FILE 'CAPLUS' ENTERED AT 08:33:56 ON 15 JUN 2007

L6 0 S L5 AND "TRANSITION TEMPERATURE"

L7 140091 S "TRANSITION TEMPERATURE"

L8 101545 S HYDRATE

L9 0 S L5 AND L8

L10 228517 S ANHYDRIDE

L11 .2184 S L8 AND L10

L12 0 S L11 AND L5

L13 0 S L5 AND PRECIPITATION

L14 0 S L5 AND PRECIPITATING

L15 0 S L5/RGT

L16 0 S L5/PREP

L17 0 S L5/PROC

L18 0 S L5/PUR

L19 0 S L5 AND PARAHYDROXYBENZOIC

FILE 'CASREACT' ENTERED AT 08:47:29 ON 15 JUN 2007

L20 0 S L5

E L5

L21 193 S E3 OR E6

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

35.02

270.53

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

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-3.12

10/553451 CRYs p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

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FILE LAST UPDATED: 13 Jun 2007 (20070613/ED)

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=> s 121
L22 193 L21

=> s 122 and 17
L23 1 L22 AND L7

=> d ibib abs

L23 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:1046581 CAPLUS
DOCUMENT NUMBER: 144:15951
TITLE: Lanthanide luminescent mesomorphic complexes with macrocycles derived from diaza-18-crown-6
AUTHOR(S): Suarez, Stephane; Mamula, Olimpia; Scopelliti, Rosario; Donnio, Bertrand; Guillon, Daniel; Terazzi, Emmanuel; Piguet, Claude; Buenzli, Jean-Claude G.
CORPORATE SOURCE: Laboratory of Lanthanide Supramolecular Chemistry, BCH 1402, Ecole Polytechnique Federale de Lausanne (EPFL), Lausanne, CH-1015, Switz.
SOURCE: New Journal of Chemistry (2005), 29(10), 1323-1334
CODEN: NJCHE5; ISSN: 1144-0546
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:15951
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Four tetracatenar (L1-L4; I, Z = CH₂, CO; R = OMe, OC₁₀H₂₁, OC₁₂H₂₅, OC₁₈H₃₃) and one hexacatenar (L5; II) ligands, derived from the diaza-18-crown-6 framework, were synthesized and characterized. In these

ligands, the amine functions are fitted with benzoxyloxybenzyl linker groups, attached either with a carbonyl function (L1) or a methylene bridge (L2-L5) and bearing alkoxy chains, R, of various lengths: R = OCH₃ for L2, OC₁₀H₂₁ for L3 and L5, OC₁₂H₂₅ for L1, and OC₁₆H₃₃ for L4. The nonmesomorphic ligands L1 and L3-L5 react with various lanthanide salts to give complexes forming thermotropic hexagonal columnar phases, as ascertained by thermal, optical and small-angle x-ray diffraction methods. The length of the alkoxy chains (L3 and L4) does not much influence the mesogenic behavior, irresp. of the linker function, the number of alkoxy chains, the counterion or the lanthanide ion. The best systems proved to be the nitrato lanthanide complexes with L3, which present a Colh phase over 100° (up to 147° for La) with melting transition temps. between 58 (La) and 86 (Tb) °C. In the case of [Eu(NO₃)₃L3], chosen as a representative example of all the complexes in this anal., the inter-column separation of 29.2 Å agrees well with the packing of cylindrical columns resulting from an alternated stacking of the mols., in which the two mesogenic arms extend on the same side, i.e. stacking the mols. in a bent conformation. The liquid crystalline phases containing Eu and Tb display metal-centered emission, meaning that these complexes are interesting building blocks for the design of luminescent liquid crystalline materials.

REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> s l22 and precipitating
 4403 PRECIPITATING
 38044 PPTG
 41354 PRECIPITATING
 (PRECIPITATING OR PPTG)
 L24 0 L22 AND PRECIPITATING

=> s l7 and l22
 L25 1 L7 AND L22

=> d ibib abs

L25 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2005:1046581 CAPLUS
 DOCUMENT NUMBER: 144:15951
 TITLE: Lanthanide luminescent mesomorphic complexes with macrocycles derived from diaza-18-crown-6
 AUTHOR(S): Suarez, Stephane; Mamula, Olimpia; Scopelliti, Rosario; Donnio, Bertrand; Guillon, Daniel; Terazzi, Emmanuel; Piguet, Claude; Buzenzi, Jean-Claude G.
 CORPORATE SOURCE: Laboratory of Lanthanide Supramolecular Chemistry, BCH 1402, Ecole Polytechnique Federale de Lausanne (EPFL), Lausanne, CH-1015, Switz.
 SOURCE: New Journal of Chemistry (2005), 29(10), 1323-1334
 CODEN: NJCHE5; ISSN: 1144-0546
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 144:15951
 GI

10/553451 CRYSTALLOGRAPHY - p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Four tetracatenar (L_1-L_4 ; I, $Z = CH_2, CO$; R = OMe, OC₁₀H₂₁, OC₁₂H₂₅, OC₁₈H₃₃) and one hexacatenar (L_5 ; II) ligands, derived from the diaza-18-crown-6 framework, were synthesized and characterized. In these ligands, the amine functions are fitted with benzoyloxybenzyl linker groups, attached either with a carbonyl function (L_1) or a methylene bridge (L_2-L_5) and bearing alkoxy chains, R, of various lengths: R = OCH₃ for L_2 , OC₁₀H₂₁ for L_3 and L_5 , OC₁₂H₂₅ for L_1 , and OC₁₆H₃₃ for L_4 . The nonmesomorphic ligands L_1 and L_3-L_5 react with various lanthanide salts to give complexes forming thermotropic hexagonal columnar phases, as ascertained by thermal, optical and small-angle x-ray diffraction methods. The length of the alkoxy chains (L_3 and L_4) does not much influence the mesogenic behavior, irresp. of the linker function, the number of alkoxy chains, the counterion or the lanthanide ion. The best systems proved to be the nitrato lanthanide complexes with L_3 , which present a Colh phase over 100° (up to 147° for La) with melting transition temps. between 58 (La) and 86 (Tb) °C. In the case of [Eu(NO₃)₃ L_3], chosen as a representative example of all the complexes in this anal., the inter-column separation of 29.2 Å agrees well with the packing of cylindrical columns resulting from an alternated stacking of the mols., in which the two mesogenic arms extend on the same side, i.e. stacking the mols. in a bent conformation. The liquid crystalline phases containing Eu and Tb display metal-centered emission, meaning that these complexes are interesting building blocks for the design of luminescent liquid crystalline materials.

REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

| => fil stng | | | |
|--|------------------|---------------|--|
| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION | |
| FULL ESTIMATED COST | 9.08 | 279.61 | |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION | |
| CA SUBSCRIBER PRICE | -1.56 | -4.68 | |

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FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Jun 8, 2007 (20070608/UP).

=> d his

(FILE 'HOME' ENTERED AT 08:28:57 ON 15 JUN 2007)

FILE 'REGISTRY' ENTERED AT 08:29:10 ON 15 JUN 2007

L1 STRUCTURE uploaded
L2 0 S L1 SSS SAM
L3 3 S L1 SSS FULL

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L4 4 S L3

FILE 'REGISTRY' ENTERED AT 08:33:14 ON 15 JUN 2007

10/553451 CRYSTAL p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

L5 1 S 61581-05-3/RN

FILE 'CAPLUS' ENTERED AT 08:33:56 ON 15 JUN 2007

L6 0 S L5 AND "TRANSITION TEMPERATURE"
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L13 0 S L5 AND PRECIPITATION
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L16 0 S L5/PREP
L17 0 S L5/PROC
L18 0 S L5/PUR
L19 0 S L5 AND PARAHYDROXYBENZOIC

FILE 'CASREACT' ENTERED AT 08:47:29 ON 15 JUN 2007

L20 0 S L5
E L5
L21 193 S E3 OR E6

FILE 'CAPLUS' ENTERED AT 08:49:45 ON 15 JUN 2007

L22 193 S L21
L23 1 S L22 AND L7
L24 0 S L22 AND PRECIPITATING
L25 1 S L7 AND L22

FILE 'STNGUIDE' ENTERED AT 08:51:44 ON 15 JUN 2007

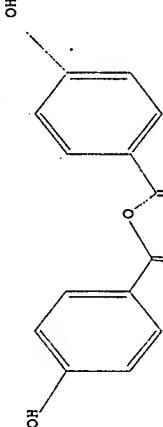
10\553451 CRYST P-HYDROXYBENZOIC ACID ANHYDRIDE - structure

=> Uploading C:\Program Files\Strucexp\Queries\2007 cases\10553451\parahydroxybenzoic anhydride.str

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11 sss sam
SAMPLE SEARCH INITIATED 08:29:33 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 849 TO ITERATE
SEARCH TIME: 00.00.01
0 ANSWERS
PROCESSED 849 ITERATIONS
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
PROJECTED ITERATIONS: 15232 TO 18728
PROJECTED ANSWERS: 0 TO 0
L2 0 SEA SSS SAM L1
=> s 11 sss full
FULL SEARCH INITIATED 08:29:42 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 17618 TO ITERATE
SEARCH TIME: 00.00.01
100.0% PROCESSED 17618 ITERATIONS
3 ANSWERS
L3 3 SEA SSS FUL L1
=> d scan

L3 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Benzoic acid, 3,4,5-trihydroxy-, anhydride (9CI)

MF C14 H10 O9

10\553451 CRYST P-HYDROXYBENZOIC ACID ANHYDRIDE - structure

=> Uploading C:\Program Files\Strucexp\Queries\2007 cases\10553451\parahydroxybenzoic anhydride.str

L1 STRUCTURE UPLOADED

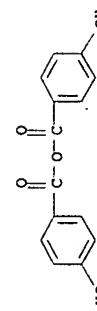
=> d 11

L1 HAS NO ANSWERS
L1 STR

** PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

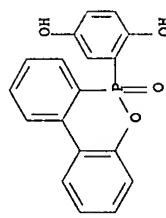
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L3 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Benzoic acid, 4-hydroxy-, anhydride (9CI)
MF C14 H10 O5
CI COM



** PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L3 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 1,4-Benzenedibasic acid, polymer with 4-hydroxybenzoic acid anhydride
and 2-(6-oxido-6H-dibenz[c,e][1,2]oxaphosphotin-6-yl)-1,4-benzenediol
(9CI)
MF (C18 H13 O4 P . C14 H10 O5 . C8 H6 O4)x
CI PMS
CM 1



CM 2

10/553431 Crys p-hydroxybenzoic acid anhydride - structure

10/553431 Crys p-hydroxybenzoic acid anhydride - structure

L4 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:26712 CAPLUS

DOCUMENT NUMBER: 134-231506

TITLE: Structure-activity relationships for the analgesic

activity of gallic acid derivatives

AUTHOR(S): Krogh, R.; Yunes, R. A.; Andricopulo, A. D.
College of Pharmacy, University of Michigan, Ann Arbor, MI, 48109, USA

SOURCE: Farmaco (2000), 55(11-12), 730-735

CODEN: FRMEB; ISSN: 0014-827X

PUBLISHER: Elsevier Science S.A.

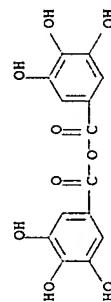
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Values of ID₅₀ for a collection of structurally-related gallic acid derivs. have been employed to create a predictive quant. structure-activity relation (QSAR) which links structure to values of analgesic activity. The QSAR model developed has substantial predictive power for the design of novel gallic acid derivs. having improved analgesic potency.

IT RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (structure-activity relationships for analgesic activity of gallic acid derivs.)

RN 330664-37-4 CAPLUS Benzoic acid, 3,4,5-trihydroxy-, anhydride (9CI) (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1987:619080 CAPLUS

DOCUMENT NUMBER: 107:213080

TITLE: Manufacture of aromatic polyester fibers

INVENTOR(S): Matsumoto, Tetsuo; Makita, Hirotoshi; Kagawa, Yoshihumi

PATENT ASSIGNEE(S): Japan Ester Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokyo Koho, 7 pp.

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

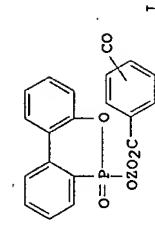
FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PATENT NO. ----- KIND ----- APPLICATION NO. ----- DATE -----

JP 62177211 A ----- JP 1986-17501 19860129

PRIORITY APPLN. INFO.: JP 1986-17501 19860129

GI



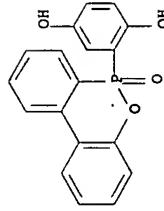
AB High-tenacity aromatic polyester fibers are prepared by melt spinning thermotropic liquid-crystalline polyesters containing 5-95 mol% I units (I = trivalent aromatic group) at draft ratio 25, passing the fibers through gas heated above the softening temperature (T_s) of the polyester, and finally passing them through gas heated above the glass transition temperature (T_g) of the polyester. Thus, a 2.5:7.5:2 (mole ratio) mixture of 9,10-dihydro-9-oxa-10-(2',5'-dihydroxyphenyl)phosphaphenanthrene 10-oxide (II), 4-hydroxybenzoic anhydride and acetic anhydride and 1 mol% terephthalic acid were copolymed, to give an aromatic polyester (III). T_s 265°; T_g 186° was spun at 330, and draft ratio 25, passed through gas at 215°, and subsequently passed through gas at 200° to give fibers with tenacity 14.7 g/denier and modulus 268 g/denier, vs. 2.8 g/denier and 205 g/denier, resp., for fibers spun at draft ratio 3.

IT 111523-01-4 RL: US5 (uses) (fiber, melt spinning of, with high tenacity and modulus, draw ratio and heat-treatment temps. in relation to)

RN 111523-01-4 CAPLUS CN 1-[4-Benzenedicarboxylic acid, polymer with 4-hydroxybenzoic acid anhydride and 2-[6-oxido-6H-dibenzo[1,2]oxaphosphorin-6-yl]-1,4-benzenediol] (9CI) (CA INDEX NAME)

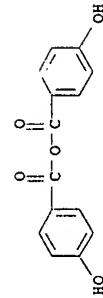
CM 1

CRN 99208-50-1 CMF C18 H13 O4 P

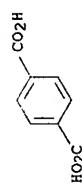


10/553451 CRYSTAL STRUCTURE OF p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

CMF C14 H10 O5



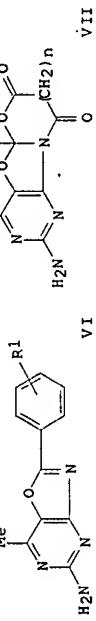
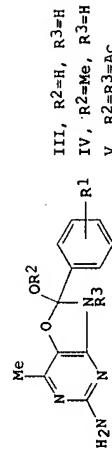
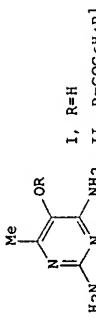
CM 3
CRN 100-21-0
CMF C8 H6 O4



L4 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1977:55385 CAPLUS
DOCUMENT NUMBER: 8655385
TITLE: Synthesis of compounds related to antitumor agents.
IV. On the reaction of aromatic carboxylates with
2,4-diamino-5-hydroxy-6-methylpyrimidine
Kato, Tetsuo; Oda, Norio; Ito, Isao
Fac. Pharm. Sci., Nagoya City Univ., Nagoya, Japan
Chemical & Pharmaceutical Bulletin (1976), 24(10),
2461-9
CODEN: CPBTAL; ISSN: 0009-2363
Journal: CPBTAL
Language: English
GI

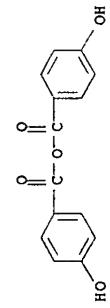
10/553451-CRYS p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

CMF C14 H10 O5



AB Reaction of the pyrimidine I with (R1C6H4CO)2O (R1 = H, OH-o, -p, Me-o, -m, -p, NO2-o, Cl-o) gave the corresponding II and the oxazopyrimidines III, III were methylated (MeI), acetylated, dehydrated, or cyclized with ClCO(CH2)NCOC (n = 1,2) to give IV-VII, resp.

IT 6581-05-3
RN RCT (Reactant); RACT (Reactant or reagent)
RN 6581-05-3 (reaction with diaminopyrimidinol)
CN Benzoic acid, 4-hydroxy-, anhydride (9CI) (CA INDEX NAME)



=> fil reg
COST IN U.S. DOLLARS
FULL ESTIMATED COST
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
CA SUBSCRIBER PRICE
TOTAL SESSION
SESSION
-3.12

SINCE FILE ENTRY
22.96
TOTAL SESSION
196.17

SINCE FILE ENTRY
-3.12
TOTAL SESSION
-3.12

FILE 'REGISTRY' ENTERED AT 08:33:14 ON 15 JUN 2007
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10/553451 CRYSTAL p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

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STRUCTURE FILE UPDATES: 14 JUN 2007 HIGHEST RN 937362-79-3
DICTIONARY FILE UPDATES: 14 JUN 2007 HIGHEST RN 937362-79-3

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TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/strogen/strodic/properties.html>

=> s 61581-05-3/rn

l5 1 61581-05-3/rn

=> d 15

l5 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN

RN 61581-05-3 REGISTRY

ED Entered STN: 16 Nov 1984

CN Benzoic acid, 4-hydroxy-, anhydride (9CI) (CA INDEX NAME)

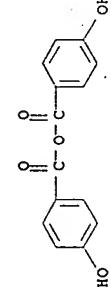
OTHER NAMES:

CN P-Hydroxybenzoic acid anhydride

MF C14 H10 O5

CI COM

LC STN Files: CA, CAPLUS, TOXCENTER



** PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplu

COST IN U.S. DOLLARS

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE ENTRY TOTAL SESSION
2.40 198.57

TOTAL

SINCE FILE

ENTRY

SESSION

TOTAL

Page 9 searched 6/15/07

10/553451 CRYSTAL p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

CA SUBSCRIBER PRICE

ENTRY 0.00

SESSION -3.12

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FILE COVERS 1907 - 15 Jun 2007 VOL 146 ISS 25
FILE LAST UPDATED: 13 Jun 2007 (20070613/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

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=> d his

(FILE 'HOME' ENTERED AT 08:28:37 ON 15 JUN 2007)

FILE 'REGISTRY' ENTERED AT 08:29:10 ON 15 JUN 2007
STRUCTURE UPLOADED
L1 0 S LA SSS SAM
L2 3 S LI SSS FULL
L3

FILE 'CAPLUS' ENTERED AT 08:31:07 ON 15 JUN 2007
L4 4 S L3

FILE 'REGISTRY' ENTERED AT 08:33:14 ON 15 JUN 2007
L5 1 S 61581-05-J/RN

FILE 'CAPLUS' ENTERED AT 08:33:56 ON 15 JUN 2007
L4 1 S 15 and "transition temperature"
1 15

988581 "TRANSITION"

26538 "TRANSITION"

1102834 "TRANSITION"

"TRANSITION" OR "TRANSITIONS")

628632 "TEMPERATURE"

81658 "TEMPERATURES"

691936 "TEMPERATURE"

("TEMPERATURE" OR "TEMPERATURES")

306948 "TEMP"

772803 "TEMPS"

3408904 "TEMP"

("TEMP" OR "TEMPS")

3568308 "TEMPERATURE"

Page 10 searched 6/15/07

```

10/553451 CRYSTAL p-HYDROXYBENZOIC ACID ANHYDRIDE - structure
          ("TEMPERATURE" OR "TEMP")
          ("TRANSITION TEMPERATURE")
L6      140091 "TRANSITION" ("TEMPERATURE")
          0 L5 AND "TRANSITION TEMPERATURE"
        => s "transition temperature"
          ("TRANSITION" OR "TRANSITIONS")
          1402834 "TRANSITION"
          ("TRANSITION" OR "TRANSITIONS")
          988581 "TRANSITION"
          264538 "TRANSITIONS"
          1102834 "TRANSITION"
          ("TRANSITION" OR "TRANSITIONS")
          629632 "TEMPERATURE"
          81658 "TEMPERATURES"
          691936 "TEMPERATURE"
          ("TEMPERATURE" OR "TEMPERATURES")
          3068348 "TEMP"
          779803 "TEMPS"
          3408304 "TEMP"
          ("TEMP" OR "TEMPS")
          3568308 "TEMPERATURE"
          ("TEMPERATURE" OR "TEMP")
          ("TRANSITION TEMPERATURE")
L7      140091 "TRANSITION" ("TEMPERATURE")
          ("TRANSITION" OR "TEMPERATURE")
        => s hydrate
          86394 HYDRATE
          28916 HYDRATES
L8      101545 HYDRATE
          (HYDRATE OR HYDRATES)
        => s 15 and 18
          1 L5
          0 L5 AND L8
        => s anhydride
          217738 ANHYDRIDE
          33390 ANHYDRIDES
L10     228517 ANHYDRIDE
          (ANHYDRIDE OR ANHYDRIDES)
        => d his
          (FILE 'HOME' ENTERED AT 08:28:57 ON 15 JUN 2007)

FILE 'REGISTRY' ENTERED AT 08:29:10 ON 15 JUN 2007
L1      STRUCTURE UPLOADED
          0 S L1 SSS SAM
          3 S L1 SSS FULL
        => FILE 'CAPLUS' ENTERED AT 08:31:07 ON 15 JUN 2007
          4 S L3
L4      FILE 'CAPLUS' ENTERED AT 08:33:14 ON 15 JUN 2007
          1 S 61581-05-3/RN
        => FILE 'CAPLUS' ENTERED AT 08:33:56 ON 15 JUN 2007
          0 S L5 AND "TRANSITION TEMPERATURE"
L5      140091 S "TRANSITION TEMPERATURE"
          101545 S HYDRATE
          0 S L5 AND L8

```

```

10/553451 CRYSTAL p-HYDROXYBENZOIC ACID ANHYDRIDE - structure
          ("TEMPERATURE" OR "TEMP")
          ("TRANSITION TEMPERATURE")
L10     228517 S ANHYDRIDE
        => s 111 and 110
          2184 L8 AND L10
        => s 111 and 15
          1 L5
L12    0 L11 AND L5
        => help operators
          The following operators are available for use in searching: 'AND', 'OR', 'NOT', '(W)', '(NOTW)', '(P)', '(NOTP)', '(S)', '(NOTS)', '(L)', '(NOTL)' and numeric operators. The order of precedence for the execution of operators is (highest first): numeric operators; '(W)', '(NOTW)', '(A)', and '(NOTA)'; '(S)' and '(NOTS)'; '(P)' and '(NOTP)'; '(L)' and '(NOTL)'; 'AND' and 'NOT'; then 'OR'. Parentheses (nesting) can be used to alter the order of execution. For example, the expression
        => SEARCH A AND B OR C NOT D
is equivalent to
        => SEARCH (A AND B) OR (C NOT D).
        If the search logic required the set 'B OR C' to be combined with set A by 'AND', logic and set D by 'NOT', logic, parentheses would be required as shown below to produce the desired results.
        => SEARCH A AND (B OR C) NOT D
For more information on the individual operators, enter "HELP" and one of the following at an arrow prompt (=>): 'NUMERIC', '(NEARLYEQUAL)', 'AND', 'OR', 'NOT', '(W)', '(P)', '(S)', '(L)', or '(NOTPROXIMITY)'. Information on specific negative proximity operators is found with the corresponding positive proximity operator; e.g., for information on '(NOTW)', enter "HELP (W)". The numeric, Boolean, and (A), (NOTA), (W), and (NOTW) word proximity operators work the same in all files. However, the function of the (S), (NOTS), (P), (NOTP), (L), and (NOTL) operators depends on the data structure of the file you are in. Entering "HELP (S)", "HELP (P)", or "HELP (L)" will give information about how these operators work in the current file.
        => d his
          (FILE 'HOME' ENTERED AT 08:28:57 ON 15 JUN 2007)
FILE 'REGISTRY' ENTERED AT 08:29:10 ON 15 JUN 2007
L1      STRUCTURE UPLOADED
          0 S L1 SSS SAM
          3 S L1 SSS FULL
        => FILE 'CAPLUS' ENTERED AT 08:31:07 ON 15 JUN 2007
          4 S L3
L4      FILE 'CAPLUS' ENTERED AT 08:33:14 ON 15 JUN 2007
          1 S 61581-05-3/RN
        => FILE 'CAPLUS' ENTERED AT 08:33:56 ON 15 JUN 2007
          0 S L5 AND "TRANSITION TEMPERATURE"
L5      140091 S "TRANSITION TEMPERATURE"
          101545 S HYDRATE
          0 S L5 AND L8

```

10/553451 CRYSTAL p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

| | COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|-----|-----------------------------------|------------------|---------------|
| L7 | 140091 S "TRANSITION TEMPERATURE" | 36.94 | 235.51 |
| L8 | 101545 S HYDRATE | | |
| L9 | 0 S L5 AND L6 | | |
| L10 | 228517 S ANHYDRIDE | | |
| L11 | 2184 S L8 AND L10 | | |
| L12 | 0 S L11 AND L5 | | |

=> s 15 and precipitation

68195 PRECIPITATION
 664 PRECIPITATION
 68699 PRECIPITATION
 (PRECIPITATION OR PRECIPITATIONS)

267038 PPTN
 4375 PPTN
 269155 PPTN
 (PPTN OR PPTNS)

291316 PRECIPITATION
 (PRECIPITATION OR PPTN)
 0 L5 AND PRECIPITATION

L13
 => s 15 and precipitating
 1 L5
 4403 PRECIPITATING
 38040 PPTG
 41350 PRECIPITATING
 (PRECIPITATING OR PPTG)

L14
 0 L5 AND PRECIPITATING
 (L5 (L) RGT/RL)

L15
 => s 15/prep
 4417183 1 L5
 0 L5/REP
 (L5 (L) PREP/RL)

L16
 => s 15/proc
 4118163 PROC/RL
 0 L5/PROC
 (L5 (L) PROC/RL)

L17
 => s 15/pur
 1 L5
 257574 PUR/RL
 0 L5/PUR
 (L5 (L) PUR/RL)

L18
 => s 15 and parahydroxybenzoic
 1 L5
 61 PARAHYDROXYBENZOIC
 0 L5 AND PARAHYDROXYBENZOIC

L19
 => fil casreact

10/553451 CRYSTAL p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

| | DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|---------------------|--|------------------|---------------|
| CA SUBSCRIBER PRICE | 0.00 | 0.00 | -3.12 |

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FILE CONTENT:1840 - 9 Jun 2007 VOL 146 ISS 25

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(FILE 'HOME' ENTERED AT 08:28:57 ON 15 JUN 2007)

FILE 'REGISTRY' ENTERED AT 08:29:10 ON 15 JUN 2007

L1
 STRUCTURE UPLOADED

L2
 0 S L1 SSS SAM

L3
 3 S L1 SSS FULL

L4
 FILE 'CAPLUS' ENTERED AT 08:31:07 ON 15 JUN 2007

L5
 4 S L3
 FILE 'REGISTRY' ENTERED AT 08:33:14 ON 15 JUN 2007

L5
 1 S 61581-05-3.RN
 FILE 'CAPLUS' ENTERED AT 08:33:56 ON 15 JUN 2007

L6
 0 S L5 AND "TRANSITION TEMPERATURE"
 140091 S "TRANSITION TEMPERATURE"

L7
 101545 S HYDRATE
 0 S L5 AND L8

L8
 228517 S ANHYDRIDE
 110 2184 S L8 AND L10
 111 0 S L11 AND L5
 112 0 S L5 AND PRECIPITATION
 113 0 S L5 AND PRECIPITATING
 114 0 S L5 AND PRECIPITATING

10/553451 CRYSTAL p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

```

L15      0 S L5/RGT
L16      0 S L5/PREP
L17      0 S L5/PROC
L18      0 S L5/PUR
L19      0 S L5 AND PARAHYDROXYBENZOIC

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FILE 'CASREACT' ENTERED AT 08:47:29 ON 15 JUN 2007

=> s 15
L20 0 L5

=> e 15
E1 1 L42N8/B1
E2 1 L42NNX2/B1
E3 166 --> L5/B1
E4 1 L50/B1
E5 1 L51784/B1
E6 27 L51787/B1
E7 1 L52/B1
E8 1 L5222/B1
E9 1 L52CU/B1
E10 1 L54KN4/B1
E11 1 L55/B1
E12 1 L56/B1

=> s e3 or e6
166 "L5"/B1
27 L51787/B1
193 "L5"/B1 OR L51787Y/B1

L21 193 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Extraction and coordination studies of the unexplored bifunctional ligand carbanoyl methyl sulfonide (CHSO_2) with uranyl(II) and cerium(III) nitrates. Synthesis and structures of $[\text{UO}_2(\text{NO}_3)_2(\text{PMSOCH}_2\text{CONBu}_2)]$ and $[\text{Ce}(\text{NO}_3)_3(\text{PMSOCH}_2\text{CONBu}_2)]$

NO HIGHLIGHTING INFORMATION PRESENT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

L21 193 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Sparsomycin analogs. V. Synthesis and antitumor activity of (E)- β -(pyrimidin-5-yl)acrylamides

NO HIGHLIGHTING INFORMATION PRESENT

L21 193 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Betaine-induced assembly of neutral infinite columns and chains of linked silver(I) polyhedra with embedded acetylendide

10/553451 CRYSTAL p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

NO HIGHLIGHTING INFORMATION PRESENT

L21 193 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Cobalt(II) and manganese(II) complexes of unsymmetric compartmental ligands bearing adjacent (H_2O) and ($\text{N},\text{S},\text{O}$) donor sets

NO HIGHLIGHTING INFORMATION PRESENT

L21 193 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Macroyclic thioether-esters and thioether-thioesters and their palladium, platinum and silver complexes

NO HIGHLIGHTING INFORMATION PRESENT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> d 121 it

L21 ANSWER 1 OF 193 CASREACT COPYRIGHT 2007 ACS on STN

IT Michaelis constant (kinetic parameters of protein kinases; preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen synthase kinase 3 inhibitors)

IT Crystal structure (of pyridocarbazole cyclopentadienyln ruthenium complex)

IT Human (preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen synthase kinase 3 inhibitors)

IT 936112-70-8P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (crystal structure; preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen synthase kinase 3 inhibitors)

IT 936112-68-4P

RL: PRP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PROC (Process) (mol. structure, HPLC chromatog. separation of isomers; preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen synthase kinase 3 inhibitors)

IT 90598-26-3

IT 114051-78-4, Lck kinase, 137632-07-6, Erk1 kinase

IT 141436-78-4, Protein kinase Ca, 144697-17-6, c-Src kinase

IT 148047-34-1, ZAP-70 kinase, 154907-65-0, 391208-93-8, Glycogen synthase kinase 3 β , Kinase 3, 433900-95-6, Glycogen synthase kinase 3 α

RL: BCP (Biochemical process); PROC (Process) (preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen synthase kinase 3 inhibitors)

IT 936233-98-3P

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

IT 85651-41-4P

IT 936112-65-1P

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

10/553451 CRYSTAL P-HYDROXYBENZOIC ACID ANHYDRIDE - structure

(preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen
synthase kinase 3 inhibitors) 80049-63-4 259752-98-2 936112-71-9
RL: RCT (Reactant); RACT (Reactant or reagent)
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen
synthase kinase 3 inhibitors) 798822-53-0P 799822-55-2P 799822-57-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen
synthase kinase 3 inhibitors)

> d his

(FILE 'HOME' ENTERED AT 08:28:57 ON 15 JUN 2007)

FILE 'REGISTRY' ENTERED AT 08:29:10 ON 15 JUN 2007
STRUCTURE UPLOADED0 S 1I SSS SAM
3 S 1I SSS FULL

FILE 'CAPLUS' ENTERED AT 08:31:07 ON 15 JUN 2007

4 S 1I 3

FILE 'REGISTRY' ENTERED AT 08:33:14 ON 15 JUN 2007.

1 S 61581-05-3.RN

FILE 'CAPLUS' ENTERED AT 08:33:56 ON 15 JUN 2007

0 S 1S AND "TRANSITION TEMPERATURE"

140091 S HYDRATE

101545 S 1S AND 1S

228517 S ANHYDRIDE

2184 S 1S AND L10

0 S 1I AND L5

0 S 1S AND PRECIPITATION

1113 S 1S AND PRECIPITATING

1114 S 1S AND RGT

1115 S 1S/PREP

1116 S 1S/PROC

1117 S 1S/PUR

0 S 1S AND PARAHYDROXYBENZOIC

1118 S 1S AND E6

1119 S 1S AND E6

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0 S 1S

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10/553451 CRYSTAL P-HYDROXYBENZOIC ACID ANHYDRIDE - structure

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> s 121
122 193 L21
> s 122 and 17
123 1 L22 AND L7
> d bib abs
L23 ANSWER 1 OF 1 CAPLUS, COPYRIGHT 2007 ACS on STN
DOCUMENT NUMBER: 20051106581 CAPLUS
144:15951
TITLE: Lanthanide luminescent mesomorphic complexes with
macrocycles derived from diaza-18-crown-6
AUTHOR(S): Suarez, Stephane; Mamula, Olympia; Scopelliti,
Rosario; Donnio, Bertrand; Buenillo, Daniel; Terazzi,
Emmanuel; Piguet, Claude; Buenillo, Jean-Claude G.;
Laboratory of Lanthanide Supramolecular Chemistry, BCH
1402, Ecole Polytechnique Federale de Lausanne (EPFL),
Lausanne, CH-1015, Switz.
New Journal of Chemistry (2005), 29(10), 1323-1334
SOURCE: CODEN: NJCHE5; ISSN: 1144-0546
Royal Society of Chemistry
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE:
LANGUAGE:
OTHER SOURCE(S): G1
CASREACT 144:13951

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
AB Four tetracatenar (L1-L4; I, 2 = CH₂, CO; R = OMe, OC10H₂₁, OC12H₂₅, OC18H₃₃) and one hexacatenar (I₂; II) ligands, derived from the diaza-18-crown-6 framework, were synthesized and characterized. In these

10/553451 CRYSTAL STRUCTURE OF p-HYDROXYBENZOIC ACID ANHYDRIDE

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT

ligands, the amine functions are fitted with benzoyloxybenzyl linker groups, attached either with a carbonyl function [L1] or a methylene bridge [L2-L5] and bearing alkoxy chains, R, of various lengths: R = OCH₃ for L2, OC₁₀H₂₁ for L3 and L5, OC₁₂H₂₅ for L1, and OC₁₆H₃₃ for L4. The nonmesomorphic ligands L1 and L3-L5 react with various lanthanide salts to give complexes forming thermotropic hexagonal columnar phases, as ascertained by thermal, optical and small-angle x-ray diffraction methods. The length of the alkoxy chains [L3 and L4] does not much influence the mesogenic behavior, irrespc., of the linker function, the number of alkoxy chains, the counterion or the lanthanide ion. The best systems proved to be the nitrate lanthanide complexes with L3, which present a Colh phase over 100° (up to 147° for L1) with melting transition temps. between 58° (L1) and 86° (mb). °C.

In the case of [Eu(NO₃)₃L3], chosen as a representative example of all the complexes in this anal., the inter-column separation of 29.2 Å agrees well with the packing of cylindrical columns resulting from an alternated stacking of the mols., in which the two mesogenic arms extend on the same side, i.e. stacking the mols. in a bent conformation. The liquid crystalline phases containing Eu and Tb display metal-centered emission, meaning that these complexes are interesting building blocks for the design of luminescent liquid crystalline materials.

REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> S 122 AND PRECIPITATING
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38044 PPGC
41354 PRECIPITATING

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L24 0 L22 AND PRECIPITATING
L25 1 L7 AND L22

=> d 1b1b abs
L25 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS ON STM
ACCESSION NUMBER: 2005:1046381 CAPLUS
DOCUMENT NUMBER: 144:15551
TITLE: Lanthanide luminescent mesomorphic complexes with
macrocycles derived from diaza-18-crown-6

Suares, Stephane; Mamula, Olimpia; Scopelliti,
Rosario; Donnio, Bertrand; Guillon, Daniel; Terazzi,
Emmanuel; Piquet, Claude; Buenzli, Jean-Claude G.
Laboratory of Lanthanide Supramolecular Chemistry, BCH
1402, Ecole Polytechnique Federale de Lausanne (EPFL),
Lausanne, CH-1015, Switz.
New Journal of Chemistry (2005), 29(10), 1323-1334
CODEN: NJCHE5; ISSN: 1144-0346
Royal Society of Chemistry
Journal
English
CORPORATE SOURCE:
CASREACT 144:15951

SOURCE:
PUBLISHER:
DOCUMENT TYPE:
LANGUAGE:
OTHER SOURCE (S):
91

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
AB Four tetracatenar [L1-L4]; I, Z = CH₂; CO; R = OMe, OC₁₀H₂₁, OC₁₂H₂₅, OC₁₈H₃₃ and one hexacatenar [L5; II] ligands, derived from the diaza-18-crown-6 framework, were synthesized and characterized. In these ligands, the amine functions are fitted with benzoyloxybenzyl linker groups, attached either with a carbonyl function [L1] or a methylene bridge [L2-L5] and bearing alkoxy chains, R, of various lengths: R = OCH₃ for L2, OC₁₀H₂₁ for L3 and L5, OC₁₂H₂₅ for L1, and OC₁₆H₃₃ for L4. The nonmesomorphic ligands L1 and L3-L5 react with various lanthanide salts to give complexes forming thermotropic hexagonal columnar phases, as ascertained by thermal, optical and small-angle x-ray diffraction methods. The length of the alkoxy chains [L3 and L4] does not much influence the mesogenic behavior, irrespc., of the linker function, the number of alkoxy chains, the counterion or the lanthanide ion. The best systems proved to be the nitrate lanthanide complexes with L3, which present a Colh phase over 100° (up to 147° for L1) with melting transition temps. between 58° (L1) and 86° (mb). °C.

In the case of [Eu(NO₃)₃L3], chosen as a representative example of all the complexes in this anal., the inter-column separation of 29.2 Å agrees well with the packing of cylindrical columns resulting from an alternated stacking of the mols., in which the two mesogenic arms extend on the same side, i.e. stacking the mols. in a bent conformation. The liquid crystalline phases containing Eu and Tb display metal-centered emission, meaning that these complexes are interesting building blocks for the design of luminescent liquid crystalline materials.

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FILE 'REGISTRY' ENTERED AT 08:29:10 ON 15 JUN 2007

L1 0 S L1 SSS SAM
L2 3 S L1 SSS FULL
L3 3 S L1 SSS FULL

L4 FILE 'CAPLUS' ENTERED AT 08:31:07 ON 15 JUN 2007
4 S L3

FILE 'REGISTRY' ENTERED AT 08:33:14 ON 15 JUN 2007

EAST Search History

W
6/18/07

| Ref # | Hits | Search Query | DBs | Default Operator | Plurals | Time Stamp |
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| L1 | 1 | p-hydroxybenzoic adj acid adj anhydride | US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT | OR | ON | 2007/06/15 09:29 |
| L2 | 1 | parahydroxybenzoic adj acid adj anhydride | US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT | OR | ON | 2007/06/15 09:29 |
| S4 | 49 | "562/895".CCLS. | US-PGPUB; USPAT; USOCR | OR | ON | 2007/06/12 20:25 |
| S5 | 144 | ((RYUZO) near2 (UENO)).INV. | US-PGPUB; USPAT; USOCR | OR | ON | 2007/01/03 11:31 |
| S6 | 301 | ((RYUZO) near2 (UENO)).INV. | EPO; JPO; DERWENT | OR | ON | 2007/01/03 11:31 |
| S7 | 49 | ((MASAYA) near2 (KITAYAMA)).INV. | US-PGPUB; USPAT; USOCR | OR | ON | 2007/01/03 11:33 |
| S8 | 91 | ((MASAYA) near2 (KITAYAMA)).INV. | EPO; JPO; DERWENT | OR | ON | 2007/01/03 11:33 |
| S9 | 6 | ((NOBUTAKA) near2 (IZUMICHI)).INV. | US-PGPUB; USPAT; USOCR | OR | ON | 2007/01/03 11:33 |
| S10 | 6 | ((NOBUTAKA) near2 (IZUMICHI)).INV. | EPO; JPO; DERWENT | OR | ON | 2007/01/03 11:33 |
| S11 | 6 | ((MASAHARU) near2 (KITTAKA)).INV. | US-PGPUB; USPAT; USOCR | OR | ON | 2007/01/03 11:33 |
| S12 | 7 | ((MASAHARU) near2 (KITTAKA)).INV. | EPO; JPO; DERWENT | OR | ON | 2007/01/03 11:34 |
| S17 | 2 | jp-2002316969-\$ did. | EPO; JPO; DERWENT | OR | ON | 2007/01/05 08:24 |
| S18 | 0 | ("2006/0264670").URPN. | USPAT | OR | ON | 2007/01/05 08:34 |
| S19 | 0 | "crystalline hydroxybenzoic acid".clm. | US-PGPUB; USPAT; USOCR | OR | ON | 2007/06/15 08:05 |
| S20 | 1317 | "hydroxybenzoic acid".clm. | US-PGPUB; USPAT; USOCR | OR | ON | 2007/06/13 07:52 |

EAST Search History

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| S21 | 49 | "562/895".CCLS. | US-PGPUB; USPAT; USOCR | OR | ON | 2007/01/05 08:36 |
| S22 | 0 | S20 and S21 | US-PGPUB; USPAT; USOCR | OR | ON | 2007/01/05 08:36 |
| S23 | 240 | S20 and granul\$ | US-PGPUB; USPAT; USOCR | OR | ON | 2007/01/05 09:01 |
| S24 | 188 | S23 and @ad<="20030417" | US-PGPUB; USPAT; USOCR | OR | ON | 2007/01/05 08:45 |
| S25 | 34 | S21 and process | US-PGPUB; USPAT; USOCR | OR | ON | 2007/01/05 08:45 |
| S26 | 2 | ("5606068").URPN. | USPAT | OR | ON | 2007/01/05 08:44 |
| S27 | 450 | S20 and precipitat\$ | US-PGPUB; USPAT; USOCR | OR | ON | 2007/01/05 09:19 |
| S28 | 357 | S27 and @ad<="20030417" | US-PGPUB; USPAT; USOCR | OR | ON | 2007/01/05 09:38 |
| S29 | 68 | S28 and granul\$ | US-PGPUB; USPAT; USOCR | OR | ON | 2007/01/05 08:58 |
| S30 | 57 | ("5025036").URPN. | USPAT | OR | ON | 2007/01/05 08:53 |
| S31 | 0 | ("6120949").URPN. | USPAT | OR | ON | 2007/01/05 08:56 |
| S32 | 141 | S28 and crystalline | US-PGPUB; USPAT; USOCR | OR | ON | 2007/01/05 08:59 |
| S33 | 0 | "para-hydroxybenzoic acid or p-hydroxybenzoic acid or parahydroxybenzoic acid".clm. | US-PGPUB; USPAT; USOCR | OR | ON | 2007/01/05 09:25 |
| S34 | 77 | "para-hydroxybenzoic acid".clm. | US-PGPUB; USPAT; USOCR | OR | ON | 2007/06/13 09:51 |
| S35 | 0 | ("4814498").URPN. | USPAT | OR | ON | 2007/01/05 09:29 |
| S36 | 1 | ("4827027").URPN. | USPAT | OR | ON | 2007/01/05 09:32 |
| S37 | 1 | ("5072036").URPN. | USPAT | OR | ON | 2007/01/05 09:33 |
| S38 | 1 | ("5532406").URPN. | USPAT | OR | ON | 2007/01/05 09:33 |
| S39 | 0 | ("6133475").URPN. | USPAT | OR | ON | 2007/01/05 09:34 |
| S40 | 2 | ("5124477").URPN. | USPAT | OR | ON | 2007/01/05 09:35 |

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| S41 | 230 | "4-hydroxybenzoic acid".clm. | US-PGPUB; USPAT; USOCR | OR | ON | 2007/01/05 10:05 |
| S42 | 183 | S41 and @ad<="20030417" | US-PGPUB; USPAT; USOCR | OR | ON | 2007/01/05 09:38 |
| S43 | 1 | ("6114157").URPN. | USPAT | OR | ON | 2007/01/05 09:48 |
| S44 | 62 | "parahydroxybenzoic acid".clm. | US-PGPUB; USPAT; USOCR | OR | ON | 2007/01/05 10:06 |
| S45 | 0 | ("2003/0160205").URPN. | USPAT | OR | ON | 2007/01/05 09:52 |
| S46 | 0 | ("6673962").URPN. | USPAT | OR | ON | 2007/01/05 09:53 |
| S47 | 0 | ("6673962").URPN. | USPAT | OR | ON | 2007/01/05 09:55 |
| S48 | 6 | "4-hydroxybenzoic acid".ti. | US-PGPUB; USPAT; USOCR | OR | ON | 2007/01/05 10:05 |
| S49 | 9 | "parahydroxybenzoic acid".ti. | US-PGPUB; USPAT; USOCR | OR | ON | 2007/01/05 10:06 |
| S50 | 14 | "para-hydroxybenzoic acid".ti. | US-PGPUB; USPAT; USOCR | OR | ON | 2007/01/05 10:06 |
| S51 | 52 | "562/895".CCLS. | US-PGPUB; USPAT; USOCR; EPO | OR | ON | 2007/06/12 20:25 |
| S52 | 1363 | "hydroxybenzoic acid".clm. | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 07:52 |
| S53 | 19107 | hydroxybenzoic adj acid | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 07:55 |
| S54 | 103853 | transition adj temperature | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 07:53 |
| S55 | 2154 | S53 and S54 | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 07:53 |
| S56 | 1164 | S55 and crystalline | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 07:54 |

EAST Search History

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| S57 | 809 | S56 and @ad<="20030417" | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 09:33 |
| S58 | 6 | hydroxybenzoic adj acid adj anhydride | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 07:55 |
| S59 | 19107 | hydroxybenzoic adj acid | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 09:33 |
| S60 | 103853 | transition adj temperature | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 09:33 |
| S61 | 2154 | S59 and S60 | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 09:33 |
| S62 | 1164 | S61 and crystalline | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 09:33 |
| S63 | 809 | S62 and @ad<="20030417" | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 09:43 |
| S64 | 466 | S63 and anhydride | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 09:34 |
| S65 | 466 | S64 and S61 | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 09:35 |
| S66 | 50 | "562/895".CCLS. | US-PGPUB; USPAT; USOCR | OR | ON | 2007/06/13 09:42 |
| S67 | 0 | S65 and S66 | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 09:34 |
| S68 | 0 | S64 and S66 | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 09:35 |

EAST Search History

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| S69 | 0 | "angle of repose" | US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT | OR | ON | 2007/06/13 09:42 |
| S70 | 8350 | angle near3 repose | US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT | OR | ON | 2007/06/13 09:42 |
| S71 | 8291 | angle near2 repose | US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT | OR | ON | 2007/06/13 09:42 |
| S72 | 3929 | S71 and @ad<="20030417" | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 09:51 |
| S73 | 0 | S63 and S72 | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 09:43 |
| S74 | 19175 | S59 or S60 and S72 | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 09:43 |
| S75 | 1164 | S74 and S62 | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 09:44 |
| S76 | 709 | S75 and anhydride | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 09:44 |
| S77 | 709 | S76 and crystalline | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 09:49 |
| S78 | 6 | hydroxybenzoic adj acid adj anhydride | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 09:47 |
| S79 | 1 | S77 and S78 | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 09:47 |

EAST Search History

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| S80 | 159 | S77 and precipitation | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 09:49 |
| S81 | 885 | "para-hydroxybenzoic acid" | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 09:51 |
| S82 | 1000 | "parahydroxybenzoic acid" | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 09:51 |
| S83 | 1206 | (S81 or S82) and @ad<="20030417" | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 09:52 |
| S84 | 2 | S83 and S72 | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 09:53 |
| S85 | 43 | S83 and S65 | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 09:54 |
| S86 | 54 | S83 and S63 | US-PGPUB; USPAT; USOCR; EPO; JPO | OR | ON | 2007/06/13 09:54 |
| S87 | 1 | "hydroxybenzoic acid anhydride". clm. | US-PGPUB; USPAT; USOCR | OR | ON | 2007/06/15 08:06 |
| S88 | 9 | ("4380587").URPN. | USPAT | OR | ON | 2007/06/15 08:06 |
| S89 | 125 | hydroxybenzoic near3 anhydride | US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT | OR | ON | 2007/06/15 08:06 |
| S90 | 75 | hydroxybenzoic near2 anhydride | US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT | OR | ON | 2007/06/15 08:16 |
| S91 | 5 | "hydroxybenzoic anhydride" | US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT | OR | ON | 2007/06/15 08:16 |

EAST Search History

| | | | | | | |
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| S92 | 0 | "parahydroxybenzoic anhydride" | US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT | OR | ON | 2007/06/15 08:16 |
| S93 | 0 | "para-hydroxybenzoic anhydride" | US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT | OR | ON | 2007/06/15 08:16 |
| S94 | 5 | hydroxybenzoic adj anhydride | US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT | OR | ON | 2007/06/15 08:18 |
| S95 | 5 | p-hydroxybenzoic adj anhydride | US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT | OR | ON | 2007/06/15 09:28 |